

Chapter 2: Spatial and Temporal Variability of Soil Processes:

Implications for Method Selection and Characterization Studies

Book Chapter --- **DRAFT**

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1.0 INTRODUCTION

The soil is a three-dimensional continuum, a temporally dynamic and spatially heterogeneous anisotropic medium comprising the outer layer of the solid earth in which liquids, gases, and solids interact over an extreme range of space and time scales. This life-sustaining open system evolves through weathering processes driven by soil formation factors: parent material, climate, organisms, and topography acting over time¹. The variation in these factors across different locations provides the soil with its inherent heterogeneity from one site to another (even for close locations). As a result, characterizing soil processes requires a capacity to consider both the mechanisms and the magnitudes of spatial and temporal variability in soil features. The magnitude of these scales may range from ion exchange and sorption reactions on the surface of kaolinite and iron oxide clay minerals, occurring at nanosecond time and microscopic scales, to the development of well-structured soil illuvial horizons and the formation of toposequences over thousands of years at the watershed scale.

Common to all these processes, and a major controlling mechanism, is the movement and redistribution of water in the soil profile. As stated by Jenny [1], “as long as water passes through the *solum*, substances are dissolved, translocated, precipitated, and flocculated, and the soil is not in a state of rest”. However, soil hydraulic properties are spatially and temporally variable. This fact is of special importance when considering the soil functional view within the environment; regulating water and solute flow and filtering organic and inorganic substances. In this regard, understanding the physical, chemical, and biological processes acting on

pollution during transport through soils is necessary to avoid further degradation of human-influenced and natural ecosystems. However, existing scientific understanding does not allow for predictions of pollution transport without *a priori* information about the soil. Even when field data are available, the applicability of models strictly depends on inherent assumptions (simplifications), as well as, the field study design, quality of the data, and perhaps most importantly, the question being asked. Thus the transfer of laboratory results or model simulations to natural systems remains a major challenge in Soil Science.

1.1 NEED FOR FIELD STUDIES

Although an academic division between those who collect field data and those who develop models often exists, it is an unnecessary partition. These two groups are interdependent as without models to compare to field data (and vice versa), the ability to improve our scientific understanding would be severely limited. While relevant studies can be performed in the laboratory or on computers, field investigations remain necessary until we can completely explain the main processes in our environment.

At the same time, field investigations are difficult, uncontrolled, time-consuming, expensive, and even dangerous. Even worse, the results of field investigations often create more questions than answers. This is both the exciting and extraordinarily frustrating activity of “field work” in Soil Science. It is also why it may be easier, or more appropriate in many cases, to satisfy a funding agency or client with modeling results.

As field studies are difficult, they require sound design to (1) meet the objectives of the study (answer the question), (2) minimize external (outside the study) influences or bias in the results, and (3) maintain a scope that falls within the limitations of space, time, and funding. It is the goal of this chapter to provide some basic considerations to meet many of these needs in field investigation design.

1.2 PRELIMINARY ISSUES

In designing field studies, three preliminary issues deserve explicit attention: questions, assumptions, and philosophical-scientific approach. Each of these three will be discussed in greater detail in the sections that follow.

Before any research can begin, defining a clear question provides the basis to consider the study design, including the operational scale, possible modeling approaches, and assumptions. The exercise of defining the study question should be clear whether (1) specific hypotheses will be tested or (2) the study is an observational investigation. The difference between hypothesis testing and observation can be blurred and are often mixed in environmental sciences. However, both have advantages and disadvantages in study design.

Hypothesis testing may be used to isolate and examine environmental processes, providing clear results or seeking concrete answers. In this approach all the factors involved in a process are controlled, except the variable under examination, identifying the effect of that variable on the process. However, it is possible that interactions between variables are unaccounted for and that the control of other variables biases the

experimental results. It is also possible (and even common) that results from field work disprove a hypothesis or show that it cannot be tested.

Observational studies include monitoring system response under ambient conditions and in response to perturbations (e.g. water or tracer additions, soil disturbance, or other alterations). These studies are excellent for determining how soil processes may change under different conditions. However, they are limited by a reduced ability to identify cause and effect in the processes under observation.

In designing either a hypothesis testing or observational study, the assumptions involved must call the researchers attention. Many fundamental assumptions of both study and model design provided by academic advisors or scientific dogma may be unconsciously incorporated into research. Assumptions in science are most often found in the form of simplifications. For example, when describing the infiltration of water through soil it is unnecessary to describe the movement of every water molecule. Instead, we describe a macro-scale process of wetting front advance. However, this simplification overlooks the importance of micro-scale interactions between water and the surfaces of solid particles such as soil aggregates. While these smaller scale processes may not be important near soil saturation, during drainage surface tension exerts greater control on the process. Therefore, an examination of the assumptions should consider what processes are being simplified and if that is justified for the question being asked.

A major scientific consideration for study design is whether the soil processes under examination are deterministic, stochastic, or complex and chaotic. This

important scientific issue, while not directly involved in a specific project, will inevitably constitute the theoretical framework influencing study design, measurement methods, as well as model selection. It could be argued that this is a physical, as opposed to philosophical, question. However the impossibility of proving such an argument requires a conceptual leap of faith.

A process is deterministic when there is a defined relationship between inputs and outputs of a system (or equation) for which there is a unique solution as in Newtonian physics. Stochasticity occurs when there is random variability in one of those inputs which results in a probability distribution of possible outcomes as opposed to a unique solution. We will define complex systems as those in which the multitude of factors in a process produce a response which may appear random, but is actually not truly random. Chaotic systems are defined as processes in which the outcome is extremely sensitive to initial conditions and sometimes they are considered a subset of complexity. The starting point may be a single number for deterministic chaos or a distribution for stochastic chaos.

A reasonable case could likely be made for one or many of these physical processes operating in any given situation. For example, water flow in porous media is represented as deterministic in the Richards equation, stochastic in the Bresler-Dagan Model, and chaotic by Faybishenko, [2], all of which will be discussed in the sections that follow. However, the researcher must select methods that inherently assume one of these scientific approaches.

Jury and Scotter [3] identified three theoretical methodologies (excluding chaos) to represent solute transport in soils: deterministic, stochastic-continuum, and stochastic-convective. Chaotic and complex processes are usually considered unpredictable over the long time scales, but this does not mean that the observations of complex and chaotic behavior are without interest. Such observations may be significant to identifying what we may be able to predict within defined space, time, and error limits and what is unpredictable with reasonable certainty.

Selection of a theoretical methodology should then be a statement of how the researcher believes nature works. A clear statement of theory for each study is directly applicable as it is a statement of assumptions often unspoken in Soil Science. It is also useful to consider whether a research-oriented or a practice-oriented model is necessary for the question being answered⁴. In some cases, simpler models have been found to adequately describe complex processes such as the transport of nitrate⁵ or pesticide occurrence in the U.S. groundwaters⁶. The selection of a practice-oriented operational model could be an attempt to avoid selecting a theoretical framework, however, pragmatism might also be considered a valid philosophy.

1.2.1 Determinism in Soil Processes

Based in Newtonian physics, deterministic systems are those with a predictable (usually unique) outcome assuming that all the factors influencing a process are included in a descriptive equation. This has been the dominant method historically in Soil Science including Darcy's law and its extension for unsaturated conditions, the

Richards equation. Most models of water and solute flow in porous media are based on Darcy's law when saturated:

$$J_w = -K_s \frac{dH}{dz} \quad (2-1)$$

and its derivative for unsaturated conditions, the Richards equation⁷:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta) \frac{\partial \theta}{\partial z} \right] + \frac{\partial K(\theta)}{\partial z} \quad (2-2)$$

In these equations J_w is the water flux, H the hydraulic head, t the time, and K is the hydraulic conductivity of the soil with the subscript s for saturated conditions and (θ) as a function of the volumetric water content at depth z . $D(\theta)$ is defined as the diffusivity or $K(\theta)\partial h/\partial \theta$, where h is the pressure head⁷. These equations of water flow provide the basis for contaminant transport analysis as the equations describing the reactions of contaminants within soil are coupled to these equations based on the law of mass conservation⁸. Solutions to the equation 2-2 are solved analytically for various boundary conditions or numerically using finite element and finite difference schemes^{8,9}.

1.2.2 Stochasticity in Soil Processes

Although it generally requires more data collection, the application of stochastic methods is becoming more common to construct spatial relationships and process models. Stochastic-continuum models use the existing deterministic equations with the hydraulic conductivity as space random functions with associated spatial relationships provided by experimental data^{10,11,12}. Stochastic characterization and hydrology will

receive more attention later in this chapter and in Chapter MM. While defining a spatial correlation function for the target variable can be difficult, this method is quite effective at describing heterogeneous media. However, it should also be recognized that while this approach transforms the deterministic Richards equation into a stochastic model by defining input parameters as random variables, the functional equation is still based on a deterministic model. This reliance on Richards equation may be a problem if transport conditions are actually chaotic^{2,13}.

Perhaps the simplest method to represent solute transport is stochastic-convective theory, or transfer function models³. This approach uses measured breakthrough curves (solute concentration measured over time under steady-state conditions) as a probability distribution of solute travel times through isolated stream tubes in a given transport volume^{3,14,15}. This so called “Black Box” methodology relies less on a mechanistic understanding of the physical processes occurring, and more on characterizing solute transport data collected at a site using transport parameters (or the 1st and 2nd centralized moments [μ & σ^2]). In this case, the breakthrough curve measured under steady-state conditions is a continuous function or the “transfer function” (TF)^{16,17}. The parameterization of a transfer function model then requires measuring a consistent transfer function, at an appropriate scale and accuracy.

Whether the study of water flow is approached under a deterministic or stochastic viewpoints can have implications for describing contaminant transport. How contaminants migrate through soil relates to the chemical, physical, and biological processes acting on solutes during transport. If solute only flows through a small

percentage of the soil, not only will the velocity be faster, but the retardation and degradation of a labile (degradable) solute will also be different. Therefore, the chemical reactions that a solute may participate in during flow through the soil cannot be correctly described unless the models describe transport pathways.

2.0 ON SPATIAL VARIABILITY

A major challenge in accurately predicting the transport of water and solutes through soils has been spatial variability or soil heterogeneity, resulting from irregularities in the soil physical structure. Among these, macropores, vertical and horizontal anisotropy (layering), and other structural soil characteristics^{18,19} have major impact. Preferential flow of solutes that results from the soil heterogeneity has been demonstrated in numerous field studies²⁰⁻²⁴.

Spatial variability has been a particular focus of Soil Science since before the classic field scale transport studies by Biggar and Nielsen [25]. Although the term, spatial variability, has been applied to explain data in many situations, there are at least five independent sources for variability observed in field studies: (1) physical heterogeneity, (2) scale differences, (3) measurement error, (4) changing boundary conditions, and (5) nonstationarity in the observed process. The latter two (4 & 5) may contribute to field observations of spatial variability, but are more correctly classified as temporal variability. Physical heterogeneity refers to the non-uniform structure of the soil. Soil is not a homogenous porous media, it is comprised of different soil layers (horizons), oddly shaped aggregates, rock fragments, cracks, plant roots, micro- and

macro invertebrate burrows, hydrophobic lenses and much more (Figure 2-1). Given this starting point, field studies also encounter variability resulting from measurements collected with different sampling volumes²⁶. As if this were not enough, measurement devices add in their own error and it is quite difficult to maintain constant boundary conditions (e.g. irrigation rate, temperature, pressure conditions, water content, tracer concentrations, and so on) during data collection periods. Finally, the dominant process may change either through deformation (changes in the physical structure) of the soil during a study or a switch in process over time. This final source of variability is nonstationarity or the lack of a consistent process response at a specific location under the same boundary conditions.

In a critical review of variability in soil processes, Jury [27] reported the static soil properties such as soil porosity, bulk density, and particle size fraction each had a coefficient of variation (variability standardized as a percent of the mean) ranging from 9% to 55%. Dynamic or process-related soil characteristics such as water and solute transport were found to have a much greater range in the coefficients of variation of 72% to 124%²⁷.

The spatial dependence of solute transport processes in the soil (scale related) has long been recognized and has been examined in numerous studies^{25,28-32}. More recently, *in situ* measurement techniques, for example time domain reflectometry (TDR), have been used to gather spatially distributed solute transport data at appropriate scales^{26,28,33,34}.

Model development, the distribution of model parameters, and estimates of parameter values must have a clear relation to the distribution of field properties³⁵. Advances toward including spatial heterogeneity found in soils into process characterization and models have been established through stochastic techniques such as Monte Carlo simulations³⁶ and geostatistical methodologies³⁷. These methods may be incorporated into models as suggested by: (1) correlating spatial associations between soil attributes and landscape factors (*i.e.* soil type, slope, aspect, vegetation...) and using these landscape factors to incorporate the dominant processes, (2) defining a variable with a population distribution assuming some spatial independence between soil attributes to perform simulations, (3) deconstructing the variability using scaling theory, (4) characterizing the spatial association between the specific soil attributes (*e.g.* semivariogram) using geostatistical tools, and (5) applying some sort of hybrid of the previous approaches^{27,38,39}.

The first of these four approaches has its greatest application in agricultural study design and statistical analyses. Through carefully designed studies that control many (if not all) environmental factors, treatments may be applied to determine how soil attributes, or processes, or both change. Results can be analyzed with analysis-of-variance techniques or statistical regression analysis, the natural (background) variability may be defined (assuming a distribution – often the normal distribution), and relationships between a location and variables like soil type, depth of water table, vegetation, or the like may be established. If this characterization occurs at the appropriate scale, the idea then is that processes in adjacent fields, or modeling cells,

may simply be summed to a total result. This type of correlation analysis in Soil Science has been called the pedotransfer function method⁴⁰. A discussion of the advantages and weaknesses of this pedotransfer functions is beyond the scope of this chapter; however, problems occur in the assumptions defining variable distributions, spatial independence, and scale.

Recently an example of the pedotransfer function method has been applied to study pesticide transport in the Central Valley of California, USA. In this case, based on the transfer function model proposed by Jury [17], different transfer functions are established for each soil type using the methods defined by Stewart and Loague [41]. Then large-scale models, that incorporate spatial variability at the scale of soil types, are used to predict pesticide leaching. Applications of the pedotransfer functions like this one have also been successful in a number of other cases^{39,40,42,43}.

The second approach involves using scaling techniques to normalize or coalesce the variability into a single characteristic or characteristic function⁴⁴. Scaling methods will be discussed in greater detail in Chapter XX.

The third approach of defining the distribution of the input variables into the models and performing a diverse range of simulations has been named Monte Carlo after the famous city of chance and gambling. Amoozegar-fard et al.[45] applied this Monte Carlo method to simulate soil solute transport, obtaining comparable results to field data. A systematic examination of the relative influence of each parameter in a model using Monte Carlo techniques is called sensitivity analyses. This technique examines how model response changes with each specific variable⁴⁶. The Bresler-Dagan

model of water and solute transport in soils is another classic example of a stochastic model that has been tested and applied in field conditions¹². In this model, the parameters for solutions of the Richards equation are defined as space random variables with statistical means and distributions defined by field measurements.

The forth approach is essentially geostatistics, which has been an area of active research, recently. More on geostatistics can be found in Chapter XYZ.

Finally combinations of these approaches exist throughout the literature. For example, Sobieraj et al. [47] recently presented a study using geostatistical techniques (semivariograms) to examine relationships between soil hydraulic conductivity (K_s) and landscape features (soil type and topography). It is interesting to note that in this paper, the authors found no relationship between the spatial structure (semivariogram) observed for K_s and either soil type or topography. They suggest that the process may be dominated by macropores and preferential flow operating on a different scale or under an alternative spatial organization. For an interesting application of most of the mentioned approaches to a single location and data set the authors recommend the papers by Keith Loague and his colleagues on the R-5 catchment⁴⁸⁻⁵⁰. These studies focused on combining an large number of infiltration measurements collected throughout a watershed into a predictive model of runoff production.

3.0 ON TEMPORAL VARIABILITY

Jenny [1] stated in his fundamental equation of soil-forming factors that the magnitude of any soil property is related to time. However, relative to the

consideration given to spatial variability, temporal variability in soil processes has received limited attention. In the case of solute transport, there are three major sources of temporal variability that include: (1) changes in the soil (or porous media) structure; (2) inconsistency in the major transport processes, and (3) changes in boundary conditions or external factors. Messing and Jarvis [51] recognized that temporal variability in soil hydraulic conductivity could result from nonequilibrium macropore flow, soil shrinking and swelling, and macropore formation and flow pathway clogging. In addition, alteration of soil macropore structure due to earthworm activity, root growth, and other bioturbation have been demonstrated to cause changes in solute transport^{21,52,53}.

Inconsistency in the major transport processes refers to a shift in the physical process controlling the flow of water and chemicals in soil. There are several distinct physical processes affecting solute transport through soil. One of these is the process of diffusion, or mass transport along a concentration gradient (Fickian diffusion), and the others are processes of advection, or mass transport along pressure (head and elevation) gradients⁸. These advective processes include: surface film flow⁵⁴, matrix flow, and preferential flow⁸. In addition to the inconsistencies of water transport, chemical nonequilibrium has the potential to produce temporal changes as chemically active sites are exhausted and molecules degrade and recombine into other molecules⁵⁵.

Finally the third, and likely most important source of temporal variability in solute transport relates to changes in the site boundary conditions including: initial water content and distribution, drainage change (perched water table or zero flux

boundary), rainfall or irrigation intensity, and other external factors (*e.g.* temperature and relative humidity).

The following examples are combinations of all three of the sources of temporal variability. The temporal variation in soil water content has perhaps been the most studied soil characteristic probably, because of the recent development of advanced measurement technologies capable of monitoring water content at high temporal and spatial resolutions⁵⁶⁻⁵⁹ (Chapter KK). Van Weesenbeck and Kachanoski, [58] demonstrated that the water profile in the first 20 cm of a cultivated soil was not stable in time. However, Vachaud et al. [59] found patterns in soil water content to have temporally stable relationships to other points in the same field. They defined time stability as the time-invariant association between spatial locations and statistical parametric values of soil deterministic properties such as texture or topography. In this regard, Kachanoski and de Jong [60] demonstrated the scale-dependent nature of time stability of soil water stored in the profile along a 720-m long soil transect. During the drying period of measurements, they observed a temporal stability across all spatial scales. However, during the wet periods, temporal stability of soil wetness was only observed for scales larger than 40 m and it was always related to the spatial pattern of the soil surface curvature across the transect. A similar finding by Comegna and Basile, [57] adds support to the observation that spatial relationships (patterns) in soil water content are temporal stability.

On the time scale of a steady-state miscible displacement, studies on temporal variability have been performed in the laboratory⁶¹, on an intact soil monolith⁶², and in a

tile drained field⁶³ to compare displacement of consecutive tracer applications to the soil surface. Although Lennartz and Kamra [61] suggested acting with prudence, these studies found temporal similarity in consecutive solute breakthrough curves. However, Campbell et al. [64] found significant variability in solute transport with time in a single plot with measurements collected at the point and plot scales. At point scale of a 3 mm diameter fiber-optic miniprobes (FOMPs)²⁶, measurements of tracer transport were consistent at some probes and wildly erratic at others. While the temporal variability at the larger measurement scale of 20 cm long TDR probes was less than that observed by the fiber optic probes, the temporal difference in measured tracer transport was still evident. The different observations by Campbell et al. [64] and Lennartz et al. [63] may be the result of different measurement scales, that Lennartz's studies were performed in a tile drained field, or simply that the results could relate to site-specific processes.

In another recent study Jaynes et al. [65] examined the consistency in the transport of pesticides and a bromide tracer in a tile drained field within a single leaching study. Consecutive pulses of bromide and pesticides were added through an irrigation system to a field scale plot (24.4 by 42.7 m) tile drained at 1.2 m depth. Similar to Campbell et al. [64], the study found that the preferential flow was not a uniform process during a constant leaching event as tracers applied later in the study had faster breakthrough times⁶⁵.

4.0 ISSUES IN FIELD STUDY DESIGN

4.1 ISSUES OF SCALE

The topic of scale has received much attention in hydrology. Although an exhaustive review is not necessary for this chapter, a brief discussion is required. For further information on this topic the readers are referred to the excellent chapters in Sposito [66] and Pachepsky et al. [67]. Many practical issues relating to the study of Soil Science involve scale, whether consciously or unconsciously included in the study design. There have been a number of attempts to define scales in hierarchical schemes based on physical features of processes⁶⁸. It has been suggested that characteristic scales may exist for specific processes.

Consider, for example, soil porosity (volume fraction void space) in a level grassland. Let us assume that we have a magic measurement system that can be applied to collect precise porosity measurements at a defined length scale over the entire surface of the grassland soil. In our experiment we start looking at the variability between individual porosity measurements for just a few adjacent measurements and then a few more increasing the combined scale of measurement. One hypothesis is that the observed variability in porosity measurements will increase until a characteristic length scale is reached, as illustrated in Figure 2-2. Then, when the characteristic length scale is exceeded (moving up a scale in Figure 2-1), the variability (in this case represented as semi-variance) will again increase until it reaches the next characteristic scale, and so on. In a hierarchical model the plateaus in Figure 2-2 would correspond to the numbered units (I.-IV.) in Figure 2-1. From aggregate to field scale, hierarchical

characteristic length scales may apply as demonstrated in the schematic diagram in Figure 2-2.

While there is some evidence for the previous discussion for *static* soil properties like bulk density⁶⁹, unfortunately, the existence of universal scales at which a multitude of *processes* in nature occur have yet to be defined or may not exist. As a consequence soil scientists have been left to heuristically defined comparable scales such as the pedon, plot, and field scales. The legacy of the limited ability of environmental scientist to standardize scales is that many studies are not quantitatively comparable.

A more reasonable set of operationally defined scales used in environmental studies have been discussed by Baveye and Boast [70] that include: “natural”, “theoretical”, “arbitrary or system”, “computational”, and “measurement” scales. These five scale classifications more or less cover all the study designs in natural sciences. Although qualitative, the value in a classification system such as this one is that scale is at least an explicit part of a study, considered in the design, even if the physical meaning of the scale classification is unknown. Each of these scale classifications will be briefly described below.

Natural scales are those based on intrinsic system properties or physical boundaries. These scales are commonly applied in the environmental sciences for example in the classic ecological hierarchy: individual, population, community, ecosystem, and landscape. The example above illustrated in Figure 2-2 would be an attempt to define natural or physically based scales. The natural scale is also the basis for defining

characteristic length scales known as Representative Elementary Volume (REV), which will be discussed in greater detail below.

Theoretical scales refer to the application of defined scales (*i.e.* meter length) in the development and applications of models. They differ from Natural scales in that they are exactly defined and applied to systems with a predefined physical relationship to process. These predefined relationships have emerged from the derivation and applications of theories to the study of the environment.

Arbitrary or System scales are dimensions or timeframes that apply to studies that are unrelated to the objective of the studies itself. These include political and property boundaries, as well as regulatory timeframes. While these scales may be very real constraints or research boundaries, they may in fact have little to do with the process under investigation.

Computational scales are again related to modeling as it refers to the discretization of time and space within models. Computational scales are often limited by computational capacity and model run time available for an examination.

Measurement scales are perhaps the most commonly encountered and an important scale to field experimental scientists. These scales are physically real boundaries of the measurement tools and the time required to collect that measurement. It is a necessity for field scientist to know the measurement scales in their studies and to report them. Measurement scales are as close to a standardization of scale as possible in the environmental sciences. This issue will also be discussed further in the following section.

4.2 CHARACTERIZING SCALE OF STUDY

All of the different scale classes mentioned above should be considered in a properly designed field study, however, two in particular deserve specific attention, – natural and measurement scales. The following discussion considers the main techniques to characterize and apply scale analysis in environmental research .

The Natural scale is most often represented in Soil Science as the Representative Elementary Volume (REV), or the minimum volume that contains all the variability in a study site^{71,72}. As this volume contains all the site variability, increasing the scale volume would not result in an increase in variability. This means that the variability would rise to a plateau as in Figure 2-2, but there after remains flat. This idea was originally developed to allow aggregation of minimum units in modeling. A conceptualization of the change in the normalized variance in a soil property with increasing volume is illustrated in Figure 2-3^{73,74}. Two experiments confirming the REV concept have been published^{73,75}, however, due to the difficulty involved, field validation of this concept has not yet been possible. Also, since each soil property manifests its own REV, a common value of REV for all kinds of observations may not exist, and a specific soil property may have different REV values in different soils⁴.

A related concept to REV exists in hillslope hydrology called the Representative Elemental Area (REA). REAs are usually much larger than REVs and refer to the minimum watershed area necessary to be able to aggregate into larger watershed models⁷⁶. It has also been argued by Baveye and Sposito [74], that the REV concept is unnecessary for modeling transport in porous media. Instead these authors propose a

relativistic continuum approach that incorporates measurement volume into macroscopic physical variables⁷⁴.

A more operationally defined REV may be based on the measurement devices used and is called the Minimum Measurement Variance Volume (MMVV)⁷⁰. A MMVV is the number of measurements using a specific technology (or the total volume of the combined measurements) that reduces the total variability to the smallest possible values. This is akin to the old-fashioned statistical estimate of the total number of samples necessary to adequately represent the mean and standard deviation (within a defined probability) for a variable of the statistical population under examination. The MMVV differs from the REV in that it is based on a combined variability of the measurement error and inherent measurement scale, whereas a true REV is based only on physical properties of the media.

Although not always explicitly stated, the MMVV methodology is commonly used to justify length scales selected for a study. For example, Campbell et al. [77] used MMVV to determine the number of 20 cm long time domain reflectometry (TDR) probes needed to characterize the vertical transport of a conservative tracer in a sloping soil. A total of 16 TDR probes were vertically inserted into a meter-squared plot on a hillslope and a tracer solution of calcium chloride was applied to the entire plot and then displaced. The temporal moments (See Appendix 1) were then estimated from the breakthrough curves. The number of TDR probes required to produce a mean within a 95% probability (that is within 10% of the “true” mean) was estimated to be 2 probes for the first moment (μ), 8 probes for the second moment (σ^2), and 22 probes for mass

recovery⁷⁷. In this case, the MMVV for μ would be 2 TDR probes for a plot of 1 by 1 m surface area and 0.2 m depth and at a confidence limit of 10%.

This example also illustrates one of the major problems in experimental characterization of MMVV scales, that is different processes are likely to have different MMVVs. The first temporal moment is mostly an advective process, the second moment includes both advection and dispersion, and the mass recovery is sensitive to advection, dispersion, and bypass flow. As a result, the estimated MMVV for each moment of the solute breakthrough curve is different.

4.3 IRRIGATION, SOLUTE DELIVERY, AND 3-DIMENSIONAL FLOW

In addition to the scale of study and measurement method (and inherent scale) another major factor in field study design is the number of dimensions over which observations will be collected. For solute transport, dimensionality means that the solute breakthrough curves will be collected in 1-D or that all three dimensions of the solute plume will be imaged. Such considerations will then influence the decision on what measurement techniques and experimental set-up, as well as models, will be most appropriate to quantify and represent the study.

The selection of the number of dimensions to include in an examination depends on the question being asked and the amount of resources available to answer that question. Not designing the dimensions (both space and time) under examination can reduce the overall effectiveness of the data. For example if the objective of the study is to observe a transient process like storm water runoff, erosion, or soil moisture then temporal resolution may be of greater importance than gathering extra spatial data.

However, observational problems may occur when using too few spatial dimensions. For example, a lysimeter installed to collect drainage from a soil pedon may only capture a limited amount of a solute tracer applied to the soil surface and leached. This low recovery of the solute mass has three possible explanations: (1) the tracer is somehow chemically active (sorbing or labile), (2) the irrigation applied was not enough to leach the solute to the depth of the lysimeter, or (3) the tracer bypassed the lysimeter by moving laterally in the soil. It should be recognized that the third result has been documented in many studies and has the potential to be common in soil solute transport^{26,78,79}. Therefore, in this example the explanatory power of the study to address the low mass recoveries is limited by the 1-D design.

It is possible in many instances to control the boundary conditions in a field plot to minimize the number of dimensions necessary to measure. The method of irrigation in solute transport studies is a common example. Irrigation methods include: flooding, various types of sprinkler irrigation, and reverse inundation (bottom to top) from some depth in the soil to the surface. The use of each of these methods will again depend on study objectives. Common to all these irrigation methods is the inclusion of a boundary layer to avoid artificial influences of the surrounding soil that is not characteristic of the designed boundary conditions. Various suggestions exist in the literature on the required dimensions of a boundary area including half the plot width. Beven et al. [80] suggested that in laboratory column studies the column diameter should be twice the length to avoid the column boundaries from influencing transport processes. Of course

such a requirement might depend upon the characteristic length scale, so no standard rule may be applied.

Examples of solute delivery as a point source, line source, or sheet source are illustrated in Figure 2-4. The careful application of these solute delivery methods can limit a study to 3-D, 2-D, and 1-D analysis, respectively. For example, Campbell et al., [81] used these different application methods as well as instrumentation designs to isolate the influence of the leaf litter layer on vertical and lateral transport in hillslope plots in a oak woodland. Without the perspectives provided by the different solute application methods and instrument designs, it would not have been possible to identify how the litter layer influences the transport processes.

Field study designs and plot characteristics for a number of investigations over the past 10- to 15 years are summarized in Table 2-1. Notice the differences in measurement techniques, plot sizes, and solute delivery for these few studies with relatively similar objectives. It is the nature of science that each study is done differently to remain unique and likely more publishable. In addition, each investigator brings their own tools and set of skills to the study design. The result, however, is that quantitative comparisons of the data from each of these studies would not be scientifically justified. Those studies using the statistical moments (μ & σ^2) to characterize BTCs have adopted a stochastic theoretical framework while others, using parameters of the convective-dispersion equation (v & D), have used a deterministic approach. Some studies include 2-D and 3-D flow while others have limited the conditions to 1-D. Finally the time scales of the study differ from days to months and

the measurement length scales range from a few to hundreds of centimeters. Any one of these differences could bias the observations for comparison with other studies, but were the appropriate designs for the original question posed by the investigator. This suggests that the greatest return can then be gained from qualitative comparisons of the soil processes.

5.0 SUMMARY AND CONCLUSIONS

It was the objective of this chapter to discuss a portion of the basic knowledge necessary for appropriate field study design in Soil Science. Focusing on soil processes, in particular solute transport, the importance of defining a clear study question, identifying the assumptions, and selecting a scientific approach were discussed. While numerous assumptions underlie our experimental and modeling methodologies in Soil Science, it is our opinion that this issue has not received the necessary attention. The alternative to selecting a particular theoretical framework is the unconscious acceptance of one provided by mentors or others in the field.

Increasing our understanding of the spatial and temporal variability of soil characteristics and processes and its application to regional and global environmental issues remains as one of the greatest challenges for future research. In particular, the description of chemical transport across scales ranging from laboratory to field or watershed is far from being reasonably successful. The interaction and inseparability of physical heterogeneity, unstable boundary conditions, scale relationships, and measurement error have limited the quantitative comparison of field studies. However,

it is not clear how to overcome these matters. As a result, scientific emphasis must remain on qualitative comparison of larger-scale process studies, along with detailed investigations of the physics of dynamic soil processes.

6.0. ACKNOWLEDGEMENTS

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7.0. APPENDIX 1: BTC DATA ANALYSIS

The tracer mass is commonly presented as the mass measured versus the mass applied, or mass recovery (M/M_o). The equation is:

$$M/M_o = \sum [C_{(z,t)} / C_o] V_w(t), \quad (2-3)$$

where $C_{(z,t)}/C_o$ is calculated for equation 2 and $V_w(t)$ is the volume of water moving past the probe during each sampling period⁸².

Moment analysis

Moment analysis is a method to quantitatively represent a statistical probability distribution using characteristic values⁸³. Although there are an infinite number of moments that may be calculated, the first two moments are usually adequate to describe statistical distributions. Using the BTCs as probability distributions of solute travel time in the soil, the first temporal moment (μ) is:

$$\mu = \int_0^{\infty} t \cdot f(t) dt, \quad (2-4)$$

where t is time on the x-axis of the BTC. This temporal moment characterizes the mean displacement time of the solute. The second temporal moment (σ^2) represents the spreading of the distribution along the x-axis. This value is defined as:

$$\sigma^2 = \int_0^{\infty} (t - \mu)^2 \cdot f(t) dt, \quad (2-5)$$

where μ is the first temporal moment and t is again time on the x-axis⁸⁴. Therefore within stochastic-convection theory, the BTCs are the relative amount of stream tubes transporting solute at a given travel time during the miscible displacement. The

moments may therefore be thought of as representing the probability distribution of these travel times over the time axis.

Temporal analysis

The Spearman's Rank test may be used to examine the temporal stability in the ranked responses measured between two BTCs^{64,59}. This test compares the ranked order of a data series for two different times or reproductions of the series. In this case, the test examines if the order of μ and σ^2 for all the probes in the first BTC is the same order measured in the second BTC. The more similar the ranked values of the two BTCs are, the closer to 1 the Spearman's coefficient will be.

Specifically, Spearman's test uses a rank R_{ij} of the measured variable (in this case μ_{ij} and σ^2_{ij}) and $R_{ij'}$, the rank of the same variable at the same location (i) at a different time (j'). The Spearman's rank correlation coefficient is:

$$r_s = 1 - \frac{6 \sum_{i=1}^n (R_{ij} - R_{ij'})^2}{n(n^2 - 1)} \quad (2-6)$$

where n is the sample size. If r_s is close to 1, the variable is temporally stable. Critical r_s values, below which the difference observed with time is considered significant, may be found in standard statistics texts⁸⁵.

Figure Captions

Figure 2-1: An example sketch of a heterogeneous field soil, with scale represented by I. Aggregate, II. Matrix, III. Pedon, and IV. Poli-pedon or Field scale classifications

Figure 2-2: Hypothetical representation of the semi-variance of soil porosity with increasing scale in a hierarchical system.

Figure 2-3: Hypothetical representation of normalized variance in a physical soil parameter up to the scale soil volume of a Representative Elementary Volume (REV).

Figure 2-4: Examples of different solute application methods to create a 1-D, 2-D, or 3-D flow plume for studies.

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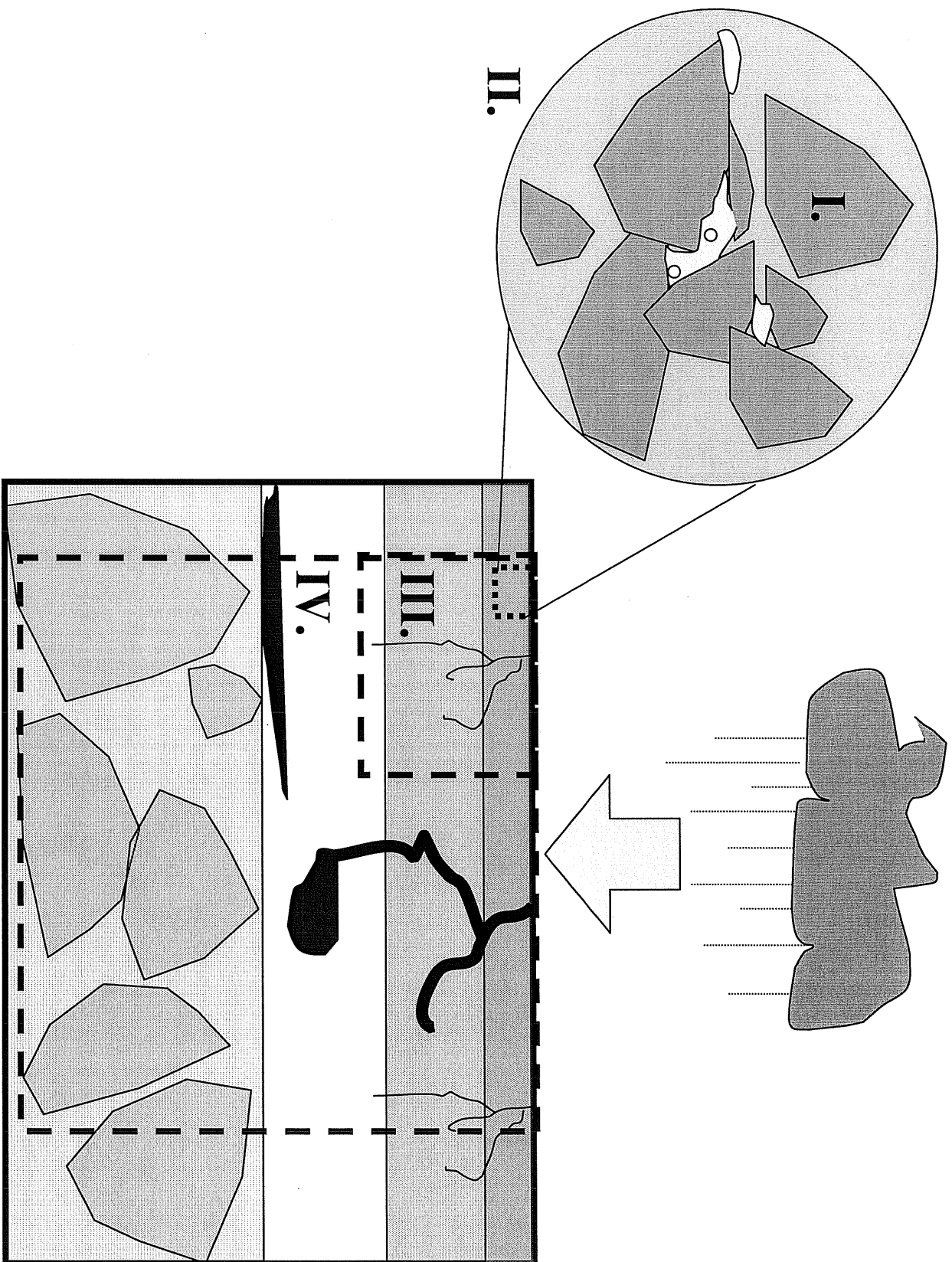


Figure 2-1

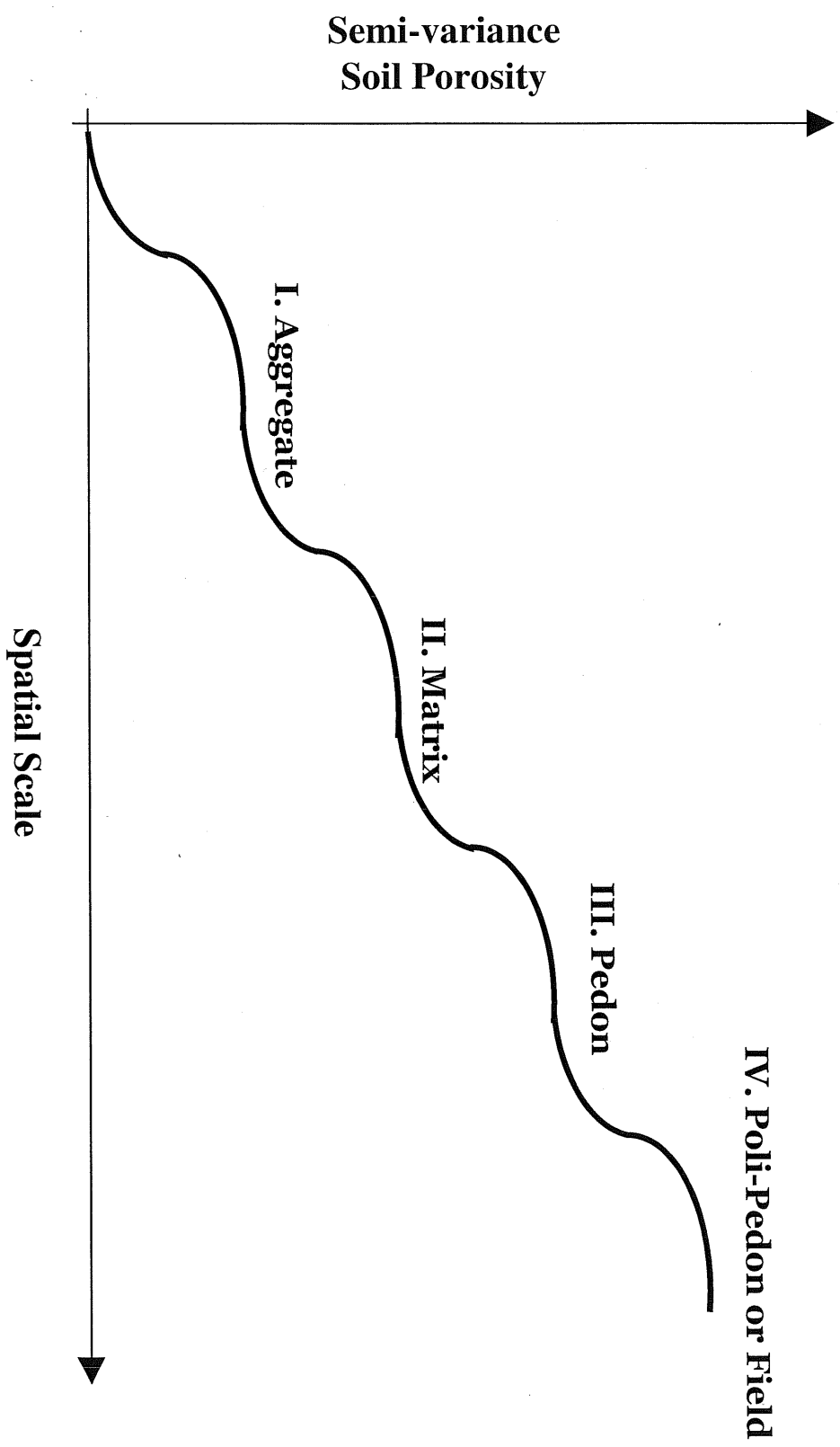


Figure 2-2

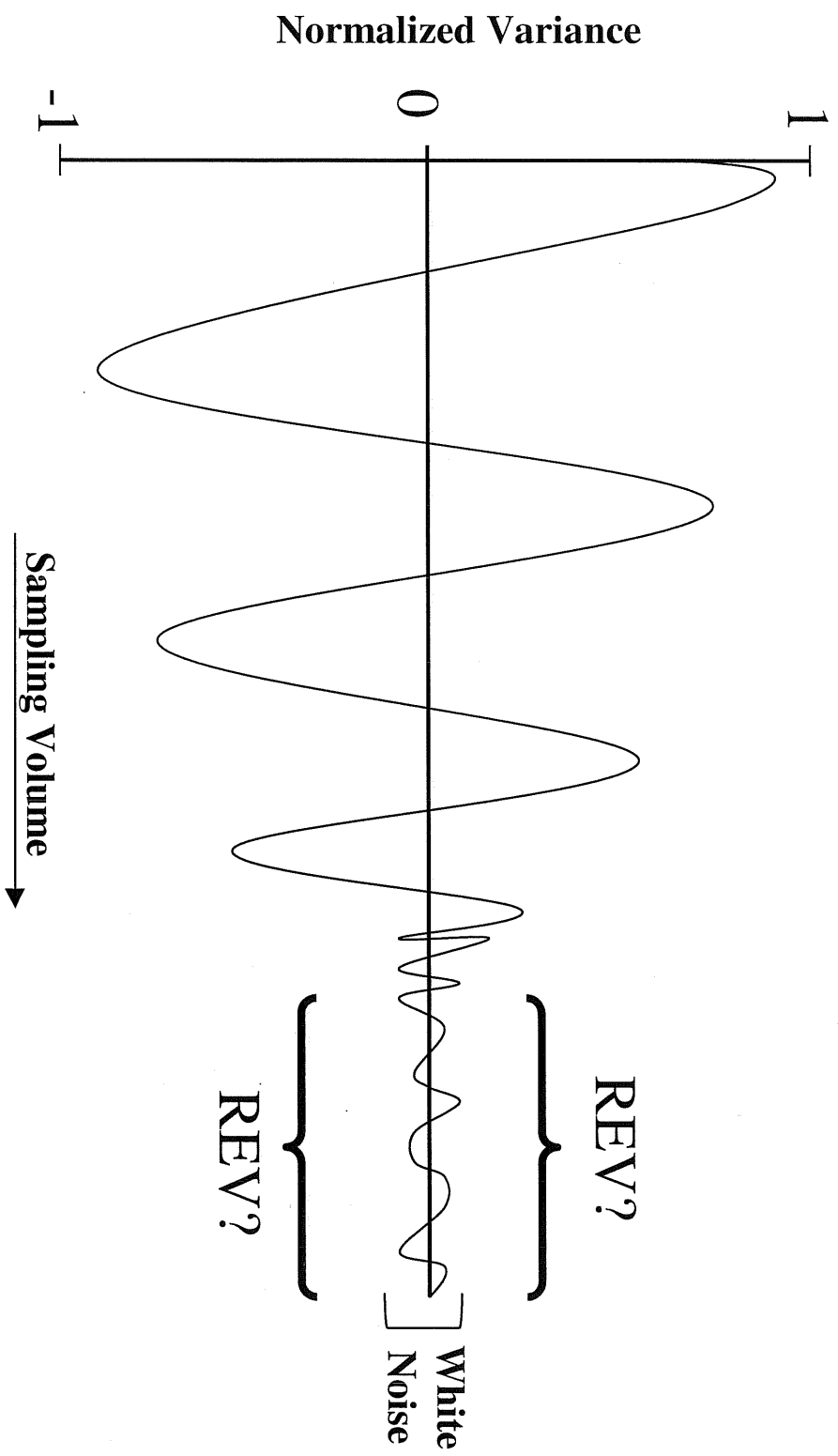
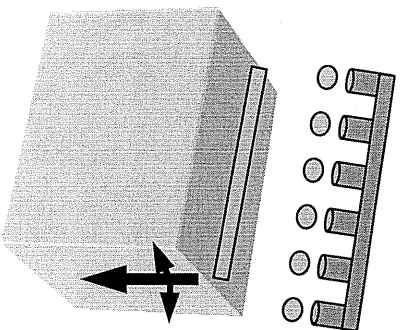
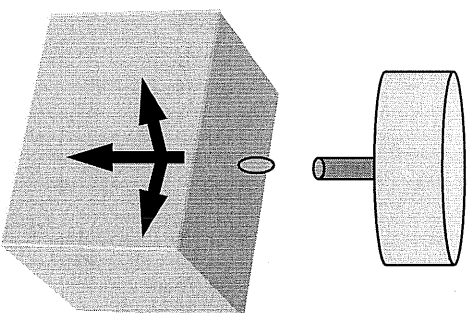


Figure 2-3

**Line Application
2-D**



**Point Source Application
3-D**



**Sheet Application
1-D**

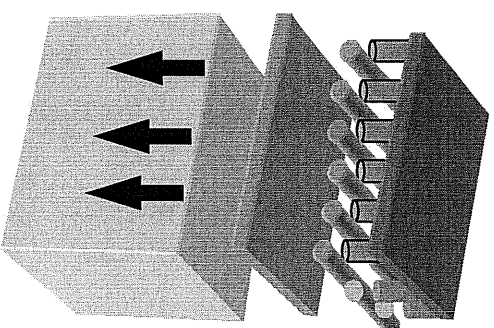


Figure 2-4

Table 1: Selected examples of field solute transport studies over the past 10-15 years summarizing study design issues

Reference	Measurement Scale	Study Length (Time)	Plot Dimensions	Soil Type	Irrigation Technique	Solute Delivery	Measuremet objectives	Boundary Area
Butters et al., (1989)	Suction lysimeters	months	80x80 m to 3.05 m depth	Typic Xeropsamment	sprinkler	same	Tracer transport and Mass recovery	Outer 60 m of plots
Campbell et al., (2002)	20 cm long TDR probes	days	3 Plots A. 1.5x1.5 m to 0.50 m depth B. 2.0x3.0 m to 0.50 m depth C. 1.0x9.0 m to 0.50 m depth	Botella Clay Loam (Pachic Argixerol)	sprinkler	A. same as irrigation B. 1-D line source 2.0 m upslope C. 1-D line source 0.50 m upslope	Tracer transport (μ , σ , Mr) inverse est.	Greater than outer 0.50 m of plot
Ellsworth et al., (1991)	6.35 cm dia. soil cores	months	2.0x2.0 to 5.0 m depth	Typic Xeropsamment	Drip irrigation	Resident concentration and sprinkler application	Tracer transport (μ , σ , Mr) inverse est.	Greater than outer 2.0 m of plot
Feyen et al., (1999)	2 m drainage troughs		13 m ² to 0.60 m depth	Umbric and mollic Gleysols	mobile spray bar	1-D line source surface and subsurface 3.3 m upslope	Tracer transport	unknown
Flury et al., (1995)	Lateral soil cores 10 cm long, 5.6 cm dia.	days	6, 1.4x1.4 m plots to 1.0 m depth	Loamy (Typic Hydraguent)and sandy (Mollic/Aquic Udifluvent)soils	mobile spray bar	Same as irrigation	Tracer and pesticide transport	Outer 0.50 m of plots
Garrido et al., (2001)	3 mm fiber optic probes 5 cm TDR probes 20 cm TDR	days	0.60x0.60 m to 0.20 m	Botella Clay Loam(Pachic Argixerol)	sprinkler	Same as irrigation	Tracer transport (μ , σ , Mr) inverse est.	Outer 0.23 m of plot
Ghodrati and Jury (1992)	7.5 cm dia., 0.5 cm long cores	week	64 , 1.5x1.5 m to 1.0 m deep plots	Tujunga loamy sand	flood & sprinkler	2-D sheet front	Pesticide mass recovery	Outer 0.25 m of each plot
Jacques et	120, 50 cm long	weeks	2 plots, 2.5x12.0 m to	Eutric Regosol	sprinkler	same	Tracer transport	Outer 1.25 m of

al., (1998)	TDR probes		.90 m depth	and Stagnic Podzoluvisol			(μ , σ , Mr) inverse est.	each plot
Jaynes and Rice (1993)	50 mm dia. suction lysimeters at 7 depths down to 3 m	months	37 m ² to 3 m depth	Avondale clay loam	Flood and drip irrigation	2-D sheet front	Tracer transport (γ , D , Mr) inverse est. CXTFIT	24 m ²
Kachanoski et al., (1992)	20 cm long TDR probes and 25 mm dia. Suction lysimeters	days	2.0x12.0 m to 0.2 m depth	Loamy sand (Typic Hapludalf)	drip	Same as irrigation	Tracer transport	unknown
Kung (1990)	Dye pattern every 25 cm ²	weeks	3.0x3.6 m to approx. 6.6 m depth	Sandy soil	precipitation and furrow flood	Furrow flood irrigation	Dye tracer transport	unknown
Mertens et al., (2002)	Single ring pressure infiltrometer (9.5 cm dia.)	days	20x80 m at surface	Luvisol sandy-loam	none	none	Hydraulic conductivity	Does not apply
Parkin et al., (1995)	0.2, 0.3, 0.4 m long TDR probes	days	2.0x2.0 m	Brunisolic Grey Brown Luvison (Typic Hapludf)	sprinkler	same	Soil moisture and hydraulic conductivity	unknown
Radcliffe et al., (1996) & Radcliffe et al., (1998)	20 cm long TDR probes, Tile drains, and soil cores (6.0-8.5 cm dia)	weeks	2 plots, 12.5x30.5 m to 1.5 m depth	Typic Kanhapludult	Sprinkler	same	Tracer transport (γ , D , Mr)	unknown
Rudolph et al., (1996)	112 suction lysimeters (2.5 cm dia.) and 168 TDR (25-200 cm)	weeks	2.0x10.0 m to 2.0 m depth	sand	Sprinkler	same	Infiltration and tracer transport	Greater than outer 0.50 m of plot
Simmonds and Norcliff (1998)	6x6 cm lysimeter	days	1.22x1.22 m to 1.0 m depth	Sandy loam	108 drip irrigation points	Same as irrigation	Tracer transport (μ , σ Mr)	Outer 0.37 m of plot